

DIFFUSION EFFECTS IN ROTATING ROTARY KILNS

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ABSTRACT

A novel approach to the modeling of mass transfer in rotary kilns has been described (Heydenrych *et al*, 2001). It considers the mass transfer to occur by the inclusion of gas in the interparticle voids in between the particles that move concentrically with the kiln. By doing so, the rate of mass transfer was found to be dependent on bed fill and the ratio of reaction rate constant to angular velocity (k/ω). The model was found to be valid at slow to medium fast reactions. For fast reactions it under-predicted mass transfer. Therefore in this paper, the model will be extended to include diffusion effects. An additional dimensionless number is necessary then to describe the system. This can either be a Peclet number ($\omega R^2/D_e$) or a Thiele modulus $(kR^2/D_e)^{1/2}$. The solution of the 2-dimensional partial differential equations that describe the extended model gives a handle on the effect of scale-up in rotary kilns. For industrial-scale kilns, the Peclet number is large, which means that diffusion within the lower (passive) layer of the bed is unimportant for slower rates. With high reaction rates, iso-concentration lines are closely stacked near the surface of the bed, implying that it is important to model the active layer rather than the bed as a whole in these circumstances. However, the stiff differential equations are not easily solved then, and other methods of solution are advisable.

Keywords rotary kiln, mass transfer, concentration profiles, effectiveness factors.

1. INTRODUCTION

Traditionally, mass transfer in rotary kilns has been modelled as a mass transfer coefficient at the surface of the bed of a rotary kiln (refs). Recently, a novel approach to the modelling of mass transfer has been suggested though (Heydenrych *et al*, 2001). This approach takes into account the inclusion of gas in the interparticle voids in between the concentrically moving particles in the passive layer of the bed. In that work, the role of the active layer where particles move along the surface of the bed was ignored by assuming that the thickness of the active layer region is infinitely thin. They concluded that their concentric movement model has merit, but that the effect of diffusion and dispersion within the bed must also be taken into account in the case of fast reactions. In this paper we will explore the effect of diffusion within the concentric flow region, and how it affects the overall mass transfer, again under the assumption of an infinitely thin active layer.

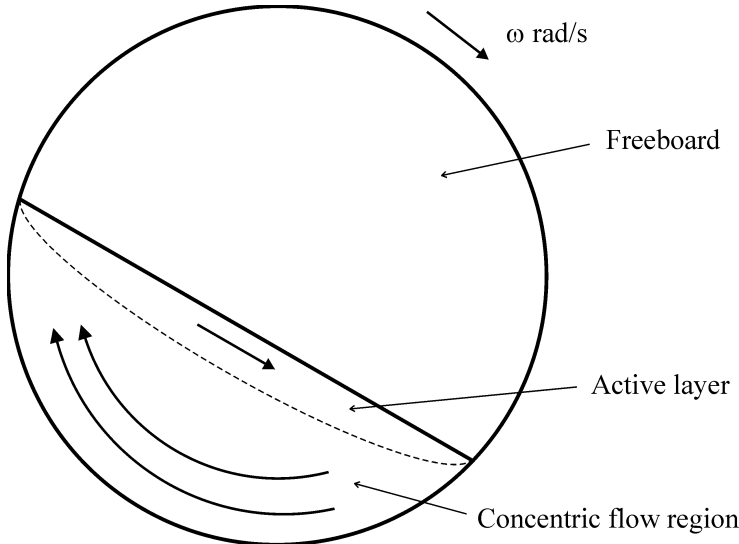


Figure 1. Shows the concentric movement and active layer regions

2. MATHEMATICAL MODEL

To take diffusion into account, consider the mass balance for a differential element within the bed (i.e. concentric flow region):

$$\frac{\partial C_A}{\partial t} = -\nabla \cdot \mathbf{N}_A + r_A \quad (1)$$

After substituting equations for the transport of gaseous A (Fick's diffusion plus convection) into the above equation, the concentration profile of A follows from

$$\frac{\partial C_A}{\partial t} = \nabla \cdot (D_e \nabla C_A - c_A \mathbf{eV}) + r_A \quad (2)$$

$$\frac{\partial C_A}{\partial t} + \mathbf{eV} \cdot \nabla C_A = D_e \nabla^2 C_A + r_A \quad (3)$$

Sharp concentration gradients are expected in the radial cross-section of kilns [Heydenrych *et al*, 2000]. In the axial direction, relatively low concentration gradients can be expected due to the high length to diameter ratio found in

typical rotary kilns. This makes it a reasonable assumption to simplify the governing equation to the two dimensions that represent the radial cross-section. Although polar coordinates may be a more natural choice of coordinate system, we have chosen rectangular coordinates because of software restrictions. Assuming steady-state operation:

$$e V_x \frac{\partial C_A}{\partial x} + e V_y \frac{\partial C_A}{\partial y} + D_e \frac{\partial^2 C_A}{\partial x^2} + D_e \frac{\partial^2 C_A}{\partial y^2} + r_A = 0 \quad (4)$$

Here, D_e is the effective diffusivity and e is interparticle voidage. Both are assumed to be constant. V_x and V_y are the x and y components respectively of the velocity of particles (and gas) in the bed, and are described by the concentric motion of the bed. Zero flux at the solid walls gives a simple boundary condition: $\vec{n} \cdot \nabla C_A = 0$ where \vec{n} denotes the normal vector at the kiln wall. For the bed surface, various boundary conditions can be used as appropriate, discussed later in the paper.

Rewriting Eqn. 4 in terms of dimensionless variables, for an n^{th} order reaction with $-r_A = ekC_A^n$:

$$\frac{1}{Pe} \frac{\partial^2 \Psi}{\partial I_x^2} + \frac{1}{Pe} \frac{\partial^2 \Psi}{\partial I_y^2} + \mathbf{u}_x \frac{\partial \Psi}{\partial I_x} + \mathbf{u}_y \frac{\partial \Psi}{\partial I_y} + \frac{ekC_{A,s}^{n-1}}{w} \Psi^n = 0 \quad (5)$$

where

$$\Psi = \frac{C_A}{C_{A,s}} \quad \text{dimensionless concentration,}$$

$$\lambda_x = \frac{x}{R}, \quad \lambda_y = \frac{y}{R}, \quad \mathbf{u}_x = \frac{V_x}{wR}, \quad \mathbf{u}_y = \frac{V_y}{wR},$$

$$Pe = \frac{e w R^2}{D_e}, \quad \text{a Peclet number modified for rotary kilns. The reaction term}$$

$\frac{ekC_{A,s}^{n-1}}{w}$ is similar to the k/ω term used by Heydenrych *et. al.* [2001] to describe concentration terms within the bed of a rotary kiln in which a first order reaction takes place.

Noting that v_x is simply the x -component of the velocity divided by the velocity at the wall, it follows from the concentric movement geometry that $\mathbf{u}_x = \mathbf{l}_y$ and $\mathbf{u}_y = -\mathbf{l}_x$ using the coordinate system given in Fig. 2. See the Appendix for more detail.

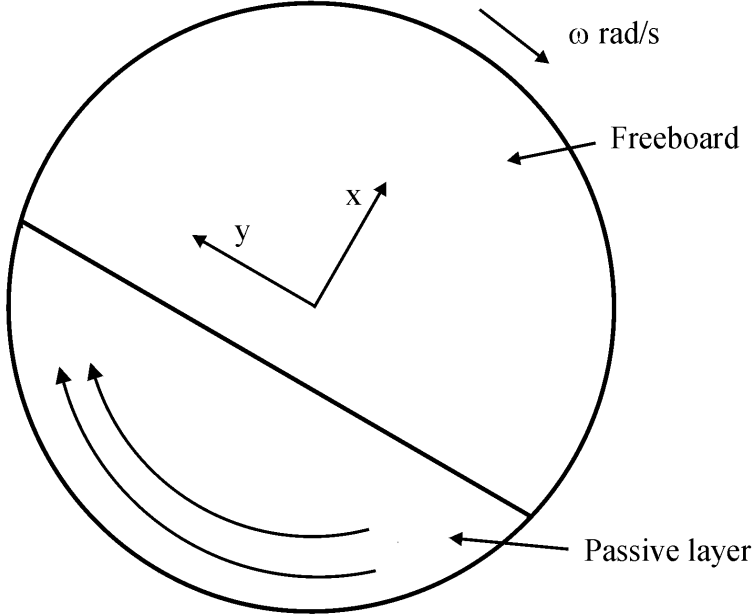


Figure 2: Applied coordinate system. We assumed that the active layer was infinitely thin.

In addition to the no-flux condition at the wall, the Danckwerts boundary condition for non-ideal flow in a plug flow reactor was used as the boundary condition at the bed surface:

$$C_{A,s} = C_A - \frac{D_e}{e V_x} \left(\frac{\partial C_A}{\partial x} + \frac{\partial C_A}{\partial y} \right) \quad (6)$$

The condition may also be written in dimensionless form as

$$\frac{\partial y}{\partial I_x} + \frac{\partial y}{\partial I_y} - Pe u_x y = -Pe u_x \quad \text{where } u_x = \frac{V_x}{Rw}. \quad (7)$$

The no-flux condition at the wall is given in dimensionless form by

$$n_x \frac{\partial \Psi}{\partial I_x} + n_y \frac{\partial \Psi}{\partial I_y} \bigg|_{I=1} = 0 \quad (8)$$

where n_x and n_y are the components normal to the wall confining the particulate solids.

The model described here (Eqns. 5, 7 and 8) is dependent on two

dimensionless variables: Pe and $\frac{kC_{A,s}^{n-1}}{w}$. Note that the square of the Thiele

modulus $f^2 = Pe \cdot \frac{kC_{A,s}^{n-1}}{w}$. This means that the system can be described by any

two of the dimensionless groups Pe , f or $\frac{kC_{A,s}^{n-1}}{w}$. In this paper we have chosen

to use $\frac{kC_{A,s}^{n-1}}{w}$ because it is the only variable that is required to describe the no-diffusion case, and Pe . The rate constant k typically changes significantly along the length of the kiln, as the solid phase approaches full conversion (or total

drying). Pe only needs to be calculated once for a given kiln because it does not typically change along the length of a rotary kiln.

Fraction fill is the third independent dimensionless variable that is necessary to describe this model. It is also interesting to note that the fraction fill does not affect the governing equations (Eqn. 5), but only the geometry of the boundary conditions.

3. SOLUTION OF THE MODEL

This model was solved using Matlab's partial differential equation toolbox. Although it would be possible to model n^{th} order reactions using the same toolbox, in this case, we have restricted our analysis to 1^{st} order reactions. For future reference, we will refer to the second dimensionless variable in its form for first-order reaction, k/ω .

The solution gives the concentration profile within the bed of the kiln, and the effectiveness factor of the bed is calculated from that concentration profile. The effectiveness factor of a rotary kiln is defined analogously to the effectiveness factor of a catalyst pellet.

$$h = \frac{-\int_V P_A dV}{-\int_V P_{A,S} dV} = \frac{-\int_V e k C_A^n dV}{-e k C_{A,S}^n V} = \frac{\int_A C_A^n dA}{C_{A,S}^n A_{bed}} = \frac{\int_A \Psi^n dA}{A_{bed}} \quad (6)$$

where $-P_A$ is the local reaction rate in the bed and $-P_{A,S}$ is the reaction rate that would occur if the entire cross section of the bed was exposed to the conditions at the surface of the bed.

For 1^{st} order reactions,

$$h = \frac{\int_A y dA}{A_{bed}}, \text{ where area } A \text{ is calculated in terms of } \lambda_x \text{ and } \lambda_y. \quad (7)$$

Given that the solution of the partial differential equation (Eq. 5) is the concentration profile over the bed, the effectiveness factor can be determined from the average dimensionless concentration over the bed cross section.

4. RESULTS AND DISCUSSION

The effectiveness factor curves for a 50%, 20% and 10% filled kiln that were generated using the model are shown in figures 3 to 6. The curve for an infinite Peclet number represents the no-diffusion case reported earlier by Heydenrych *et. al.*, 2001.

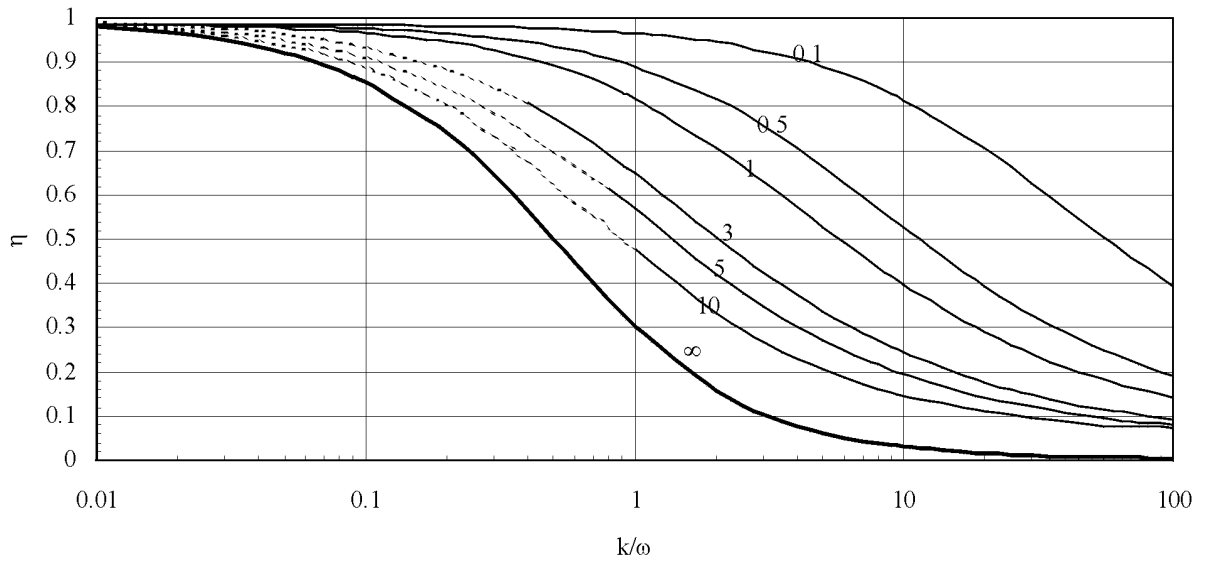


Figure 3: Effectiveness factors as a function of k/ω for a 50% filled kiln; 1st order reaction.

As expected, the inclusion of diffusion effects in the model increases the effectiveness factor in all conditions. It should also be noted that for a given Peclet number (i.e. kiln size and rotation speed), the effect of diffusion as a *fraction* of the contribution by gas inclusion, is far higher at high values of k/ω , where high concentration gradients occur in the bed (predominantly near the surface of the bed). For commercial scale rotary kilns, Peclet numbers are typically greater than 1000, discussed later in the paper.

At higher Peclet numbers ($Pe > 10$), the numerical method was unable to converge on a solution. The dashed lines on Figure 3 are extrapolations, where the model failed to solve. A possible reason for the poor convergence of the model at large Peclet numbers, is that the numerical methods used to solve the model were based on techniques suited for an elliptical (second-order) partial differential equation, with the first-order term simply being handled as a source term. At high Peclet numbers, the second-order terms of the partial differential equation become less important, and the numerical method is unsuited to the solution of what effectively becomes a first-order hyperbolic pde that dominates the model.

Similar solutions have been found for kilns with bed fills of 20% and 10% (Figs. 4 and 5 respectively)

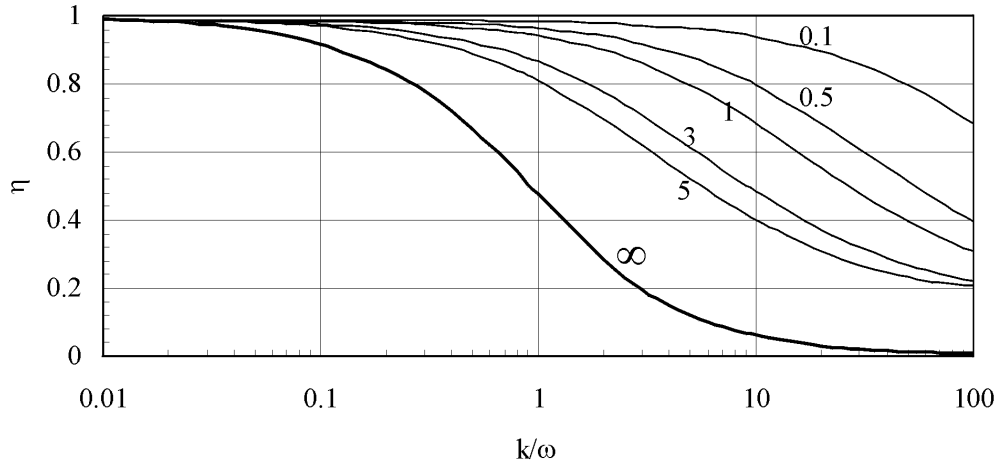


Figure 4: Effectiveness factors as a function of k/ω for a 20% filled kiln; ; 1st order reaction.

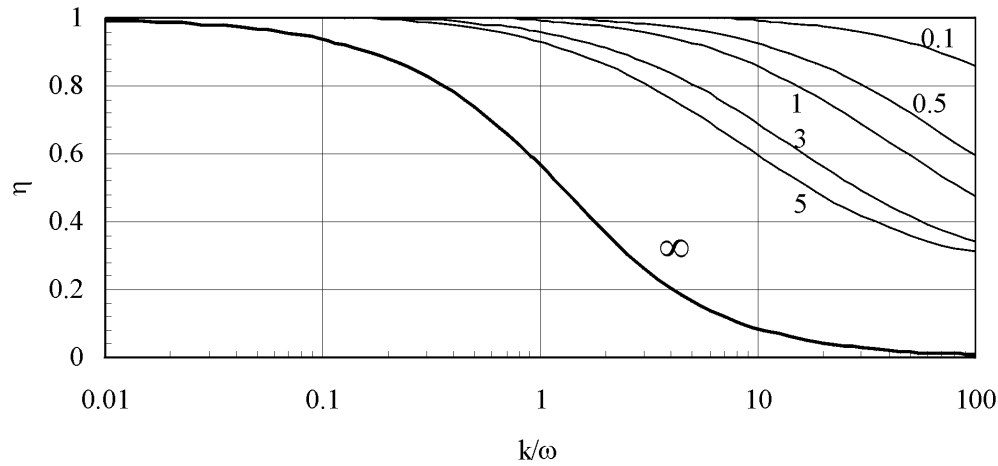


Figure 5: Effectiveness factors as a function of k/ω for a 10% filled kiln; 1st order reaction.

As the fill fraction decreases, the effect of diffusion appears to become more important. The concentration profiles generated at certain Pe and k/ω values are interesting, and are shown in Fig. 6 for a half-filled kiln:

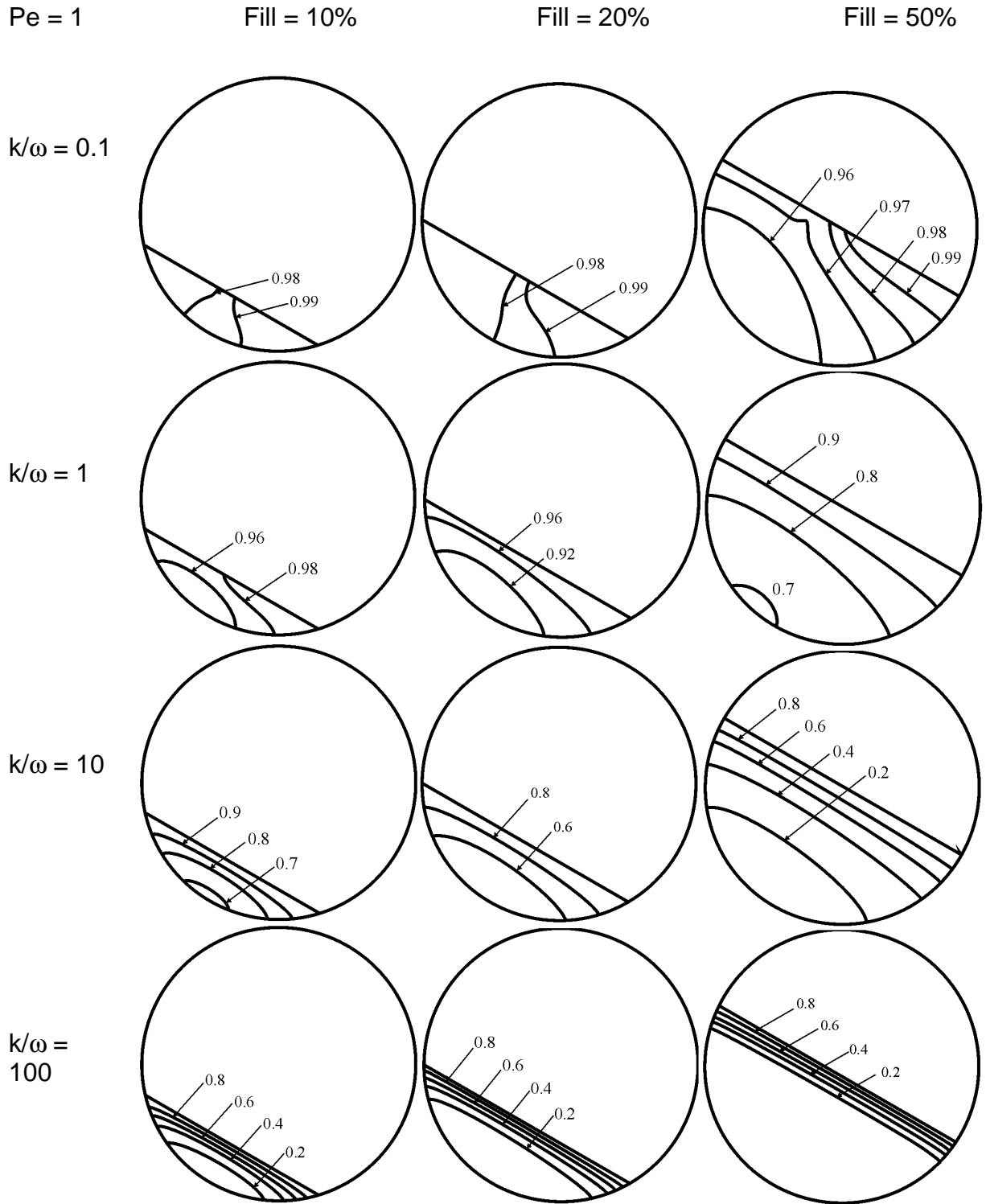


Figure 6: Concentration profiles at $Pe = 1$; 1st order reaction.

The straight iso-concentration lines predicted for the no-diffusion case (Heydenrych *et. al*, 2001) are only readily evident for the diagram where $k/\omega = 0.1$. For the other cases, diffusion effects dominate the shape of the concentration profile, and the rotation of the kiln does not distort the profile significantly.

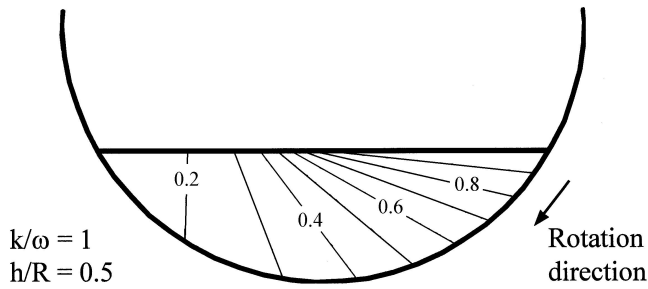


Figure 7. If diffusion is not taken into account, straight iso-concentration lines are expected.

5. SCALE-UP EFFECTS

The models have shown that for Peclet numbers less than 100, diffusion effects are important. But under what circumstances can we expect such low Peclet numbers, and what Peclet numbers are typical for rotary kilns?

The diffusivities of a gas at atmospheric pressure vary between 10^{-4} - 10^{-6} m²/s (Knudsen *et al.*, 1997). Values of 2×10^{-4} m²/s, 2×10^{-5} m²/s and 2×10^{-6} m²/s were used to for the diffusivity of the reactant gas D_A .

The effective diffusivity in the bed of the kiln can be estimated as follows:

$$D_e = \frac{D_A \epsilon}{\tau} \text{ (Knudsen *et al.*, 1997)}$$

Using a tortuosity (τ) of 2 and voidage (ϵ) of 0.5, we can expect effective diffusivities within the bed of 5×10^{-5} m²/s (max.), 5×10^{-6} m²/s and 5×10^{-7} m²/s (min.).

Kiln rotation speeds vary less, because at lower rotation speeds, slumping of the bed can occur. At higher rotation speeds, centrifugation begins. For this reason, only two angular velocities are considered, 0,5 rad/s and 0,1 rad/s.

The effect of scale is largely dependent on the radius, because $Pe \propto R^2$. Table 1 shows Peclet numbers for selected D_e and ω values as a function of radius.

Table 1. Peclet numbers for typical rotation speeds and effective diffusion coefficients. Cells with $Pe < 1000$ are not shaded to indicate that this only occurs in laboratory-scale kilns with high D_e values.

	D_e , m ² /s	5×10^{-5}		5×10^{-6}		5×10^{-7}	
		ω , rad/s		ω , rad/s		ω , rad/s	
radius (m)	0.05	0.1	0.5	0.1	0.5	0.1	0.5
	0.1	5	25	50	250	500	2500
	0.5	20	100	200	1000	2000	10000
	1	500	2500	5000	25000	50000	250000
	5	2000	10000	20000	100000	200000	1000000
		50000	250000	500000	2500000	5000000	25000000

As an example, the Peclet numbers for the rotating drum used by Jauhari *et al* (1998), with a rotating drum of radius 0.145 m, varies from 530 to 3600,

depending on rotation speed. It is obvious that diffusion as a possible extra transport mechanism to gas entrapment can safely be neglected for practical applications as well as for most lab experiments.

6. CONCLUSIONS

A mathematical model has been presented that improves on the previous model (Heydenrych *et al*, 2001) by adding diffusion effects to gas entrapment in the concentric flow region of a rotary kiln. The technique, but not the model, is limited to moderate Pe numbers. For practical values of Pe, a modified solution technique is required. Heydenrych *et al*, 2001 have shown that k/ω is the parameter that describes mass transfer at low to moderate reaction rates. In this paper, Peclet number was implemented (in addition to k/ω) to model diffusion effects. This number is defined as $\omega R^2/D_e$. The Peclet number provides a tool for predicting scale-up effects, and even though the model presented here is oversimplified due to the assumption of an infinitely thin active layer, it nevertheless provides an insight to the use of the Peclet number for the scale-up of rotary kilns.

Diffusion in the concentric flow region was found not to add much to the mass transfer at realistic conditions where the Peclet number is much higher than 1. At high k/ω values, however, concentration gradients become fully concentrated near the surface of the bed, and here the assumption that the active layer is infinitely thin becomes a poor assumption as all mass transfer is occurring within this layer. This model shows that the entrapment of gas perpendicular to the bed is relatively unimportant compared to diffusion effects at these higher k/ω values.

Further work should be concentrated at developing a suitable model for the active layer, where a 1-dimensional dispersion model would be a fair assumption, based on the results of this work. It will also be important to determine the depth of the active layer, and how the movement of particles over each other affects the dispersion of the gas in the direction perpendicular to the bed surface. This information will give the boundary conditions for the concentric flow region, with the aim of generating a comprehensive model including all mechanisms for mass transfer.

7. ACKNOWLEDGEMENT

The useful contribution of Angela Smith in documenting the work presented here, is gratefully acknowledged.

Symbol	Units	Description
A	m^2	Cross sectional area of the bed of the rotary kiln
C_A	kmol.m^{-3}	Concentration of reactant A in the bed of the rotary kiln
$C_{A,s}$	kmol.m^{-3}	Concentration of reactant A at the surface of the bed
D_e	$\text{m}^3.\text{s}^{-1}$	Effective diffusivity of reactant A
Pe		Peclet number modified to suit a rotary kiln
R	m	Radius of kiln
r	$\text{kmol. m}^{-3}.\text{s}^{-1}$	Reaction rate of a reactant A
V	m/s	Velocity of gas within the bed
x		Co-ordinate in x direction
y		Co-ordinate in y direction

Greek Letters

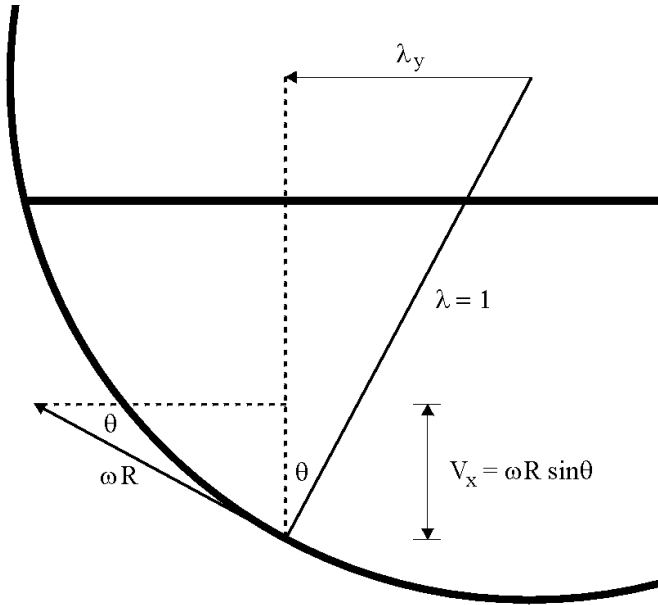
ε		Voidage of the bed of the rotary kiln
ϕ		Thiele modulus
η		Effectiveness factor
λ		Dimensionless distance
τ		Tortuosity
u		Dimensionless velocity
ω	rad/s	Angular velocity of kiln
ψ		Dimensionless concentration

8. REFERENCES

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APPENDIX

Proof that $u_x = l_y$ and $u_y = -l_x$



Consider a point on the radius, which is at $\lambda = 1$ in dimensionless coordinates. By definition,

$$u_x = \frac{V_x}{\omega R}$$

Substituting for V_x ,

$$u_x = \frac{\omega R \sin \theta}{\omega R} = \sin \theta$$

From the diagram,

$$l_y = \sin \theta = u_x$$

At points away from the wall, u_x and λ_y decrease proportionately. It can similarly be shown that $u_y = -l_x$.